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SCIATRAN 2.0 – A new radiative transfer model for geophysical applications in the 175–2400 nm spectral region

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Abstract

A successor version of the SCIATRAN radiative transfer model (RTM) has been developed to perform radiative transfer modeling in any observation geometry appropriate to measurements of the scattered solar radiation in the Earth's atmosphere. The model is designed to be used as a forward model in the retrieval of atmospheric constituents from measurements of scattered solar light by satellite, ground-based, or airborne instruments in UV–Vis–NIR spectral region. Furthermore, it can be used to calculate air mass factors or fluxes. The new generation of the SCIATRAN model comprises all features of the latest SCIATRAN 1.2 RTM supporting additionally radiative transfer calculations in a spherical atmosphere. The program is written in FORTRAN 95 and suitable for parallel execution using the OpenMP standard. The wavelength range covered by the radiative transfer model is extended to 175–2380 nm including Schuman-Runge and Herzberg absorption bands of oxygen. The SCIATRAN 2.0 model exhibits the following new capabilities: (i) modeling of the scattered solar radiation in limb viewing geometry as well as any kind of measurements of the scattered radiation within the atmosphere, (ii) corresponding quasi-analytical calculation of weighting functions of atmospheric parameters, (iii) airmass factor calculations for ground-based, space and airborne measurements including off-axis geometry, (v) accounting for photochemically active species, i.e., radiative transfer calculations can be performed using solar zenith angle dependent vertical distributions of atmospheric species, (iv) height resolved radiation fluxes, including actinic fluxes for photolysis rate calculations, (vi) inelastic rotational Raman scattering in any supported viewing geometry, (vii) new effective approximations for radiative transfer modeling in presence of clouds. The SCIATRAN model is freely available via the world wide web for non-commercial scientific applications.

Keywords: Radiative transfer model; Terrestrial atmosphere; Spherical geometry; Ultraviolet; Visible; Near-infrared

1. Introduction

The SCIATRAN radiative transfer models (RTMs) are next generation RTMs based on the well-known GOMETRAN (Rozanov et al., 1997) model which was originally developed to simulate solar radiation backscattered from the atmosphere and reflected from the Earth's surface in the spectral range 240–800 nm as measured by the Global Ozone Monitoring Experiment (GOME) in nadir viewing geometry. A successor RTM called SCIATRAN (Rozanov et al., 2002) was extended to cover the spectral range 240–2380 nm comprising the eight spectral channels of the SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) instrument. SCIATRAN versions up to 1.2 utilize the pseudo-spherical approach, including refraction, appropriate for solar zenith angles up to about 92° and near-nadir viewing angles.

A new generation of the SCIATRAN model comprises all features of the latest SCIATRAN 1.2 RTM

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supporting additionally radiative transfer calculations in a spherical atmosphere (Rozanov et al., 2001). The program is written in FORTRAN 95 and suitable for parallel execution using the OpenMP standard (OpenMP, 1997–2004). The wavelength range covered by the radiative transfer model is extended to 175–2380 nm including Schuman-Runge and Herzberg absorption bands of oxygen. The SCIATRAN 2.0 model exhibits many new capabilities making it valuable for a wide range of scientific applications.

2. Main features

Due to a newly implemented spherical mode and an improved plane-parallel mode, the SCIATRAN radiative transfer model becomes suitable to solve almost any scientific task associated to measurements of the scattered solar radiation in the Earth's atmosphere in the ultraviolet, visible, and near-infrared (UV–Vis–NIR) spectral regions. The radiative transfer modeling can be performed at any viewing geometry common for measurements of the scattered solar radiation within or above the atmosphere, e.g., limb, nadir, off-nadir, zenith, or off-axis as measured by satellite, air- and balloon-borne, or ground-based instruments, for a wide range of solar zenith angles. The SCIATRAN radiative transfer model can be operated either in the plane-parallel mode ignoring the sphericity of the Earth's atmosphere and performing all radiative transfer calculations in a plane-parallel media or in the spherical mode properly accounting for the spherical shape of the Earth's atmosphere. In the spherical mode the Earth's atmosphere is considered to be symmetrical with respect to the solar principal plane allowing the solar zenith angle dependent composition of the atmosphere to be accounted for. The surface reflective properties can be described by either constant or wavelength dependent lambertian albedo in both plane-parallel and spherical modes as well as by the bidirectional reflectance distribution function (BRDF) using a pre-calculated data base for various surface types in the spherical mode.

As a standard method to solve the integro-differential radiative transfer equation in a plane-parallel atmosphere the discrete-ordinates method (Stamnes et al., 1988; Siewert, 2000) is employed. To calculate the outgoing radiance at the top of the atmosphere either the finite difference scheme (Rozanov et al., 1997) or the finite element approach (Samarskij, 2002) can be used in the framework of the SCIATRAN 2.0 radiative transfer model alternatively to the discrete-ordinates method. The plane-parallel mode is commonly used at line-of-sight zenith angles $\lesssim 30°$ and may result in significant errors at larger angles depending on the solar zenith angle, wavelength, and optical properties of the atmosphere, see Rozanov et al. (2000) for details. An ordinary plane-parallel approach is only valid for solar zenith angles less than 90°. This limitation can be avoided employing the pseudo-spherical extension (Rozanov et al., 2002), i.e., calculating the light paths for the direct solar beam in a spherical atmosphere and then solving the plane-parallel radiative transfer equation.

In the spherical mode the combined differential-integral (CDI) approach is employed (Rozanov et al., 2001), i.e., an integral radiative transfer equation is solved properly accounting for the single scattering in a spherical atmosphere and using an approximation for the multiple scattering. At the first step an approximate spherical solution is obtained calculating the multiple scattering source function employing the solution of the integro-differential radiative transfer equation in a plane-parallel atmosphere. If required, this solution can be improved using a subsequent iterative approach also known as the Picard iterative approximation. This iterative approach resulting in the fully spherical solution is referred to as the CDIPI model. Any viewing geometry and solar zenith angles up to 98° are supported. In atmospheric layers intersected by the line-of-sight at local solar zenith angles larger than 98° the contribution of the multiple scattering into the total source function is set to zero.

An extensive comparison of outgoing radiances in limb viewing geometry simulated by five different radiative transfer models including the approximative spherical CDI model and the fully spherical CDIPI model which are parts of SCIATRAN 2.0 was performed by Loughman et al. (2004). The comparison demonstrates a good agreement between the spherical models under ordinary conditions.

Fig. 1 shows the outgoing radiation at the top of the atmosphere as a function of the wavelength and of the viewing angle at a solar zenith angle of 89° computed in plane-parallel and spherical modes. Positive viewing angles correspond to the solar direction, i.e., the radiance is simulated assuming a detector looking in the solar principal plane towards the Sun, and negative values denote the anti-solar direction. As clearly seen, employing the plane-parallel approach the outgoing radiance detected in the anti-solar direction is strongly overestimated whereas an underestimation occurs when looking toward the Sun.

The SCIATRAN 2.0 radiative transfer model is linearized with respect to atmospheric trace gas number densities in both spherical and plane-parallel modes and, additionally, with respect to many other important atmospheric parameters (e.g., pressure, temperature, Rayleigh scattering coefficient, aerosol and cloud parameters, etc.) in the plane-parallel mode. The weighting functions are calculated employing the quasi-analytical approach discussed by Rozanov et al. (1998). Figure 2 shows a comparison of normalized ozone weighting functions in limb viewing geometry at 20 km tangent

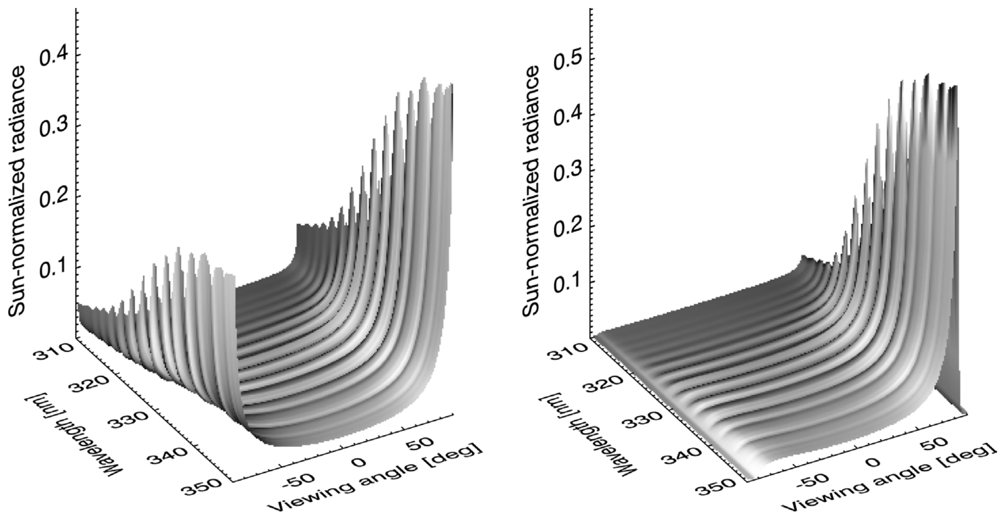

Fig. 1. Outgoing radiation at the top of the atmosphere as a function of the wavelength and of the viewing angle at a solar zenith angle of 89° in plane-parallel (left plot) and spherical (right plot) modes. Positive viewing angles correspond to the solar direction and negative values denote the anti-solar direction.

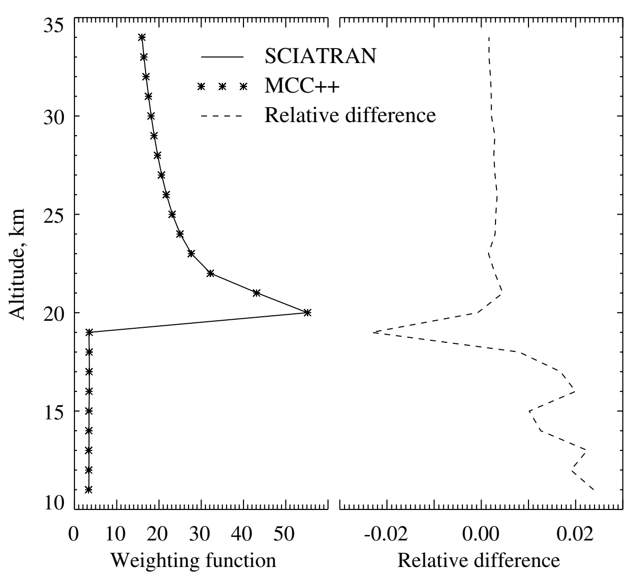

Fig. 2. Normalized ozone weighting functions at a wavelength of 600 nm in limb viewing geometry at 20 km tangent height and a solar zenith angle of 40° as calculated by SCIATRAN and MCC++ radiative transfer models and the corresponding relative difference (SCIATRAN – MCC++)/MCC++.

height at a wavelength of 600 nm as calculated by SCIATRAN and the Monte Carlo model MCC++ (Postylyakov, 2004). As seen from the plot, the weighting functions resulting from the different models agree within 0.5% down to the maximum and differ by at most 2.5% below.

Beside the radiance and weighting functions, the SCIATRAN radiative transfer model can also be used to calculate air mass factors for satellite, ground-based, and airborne measurements including off-axis geometry as well as height resolved radiation fluxes including actinic fluxes needed for photolysis rate calculations under both daylight and twilight conditions. To allow for ozone photolysis rate calculations, the wavelength range covered by the radiative transfer model was extended to 175–2380 nm including Schuman-Runge and Herzberg absorption bands of oxygen shown in Fig. 3. The spectral convolution of the radiance shown in Fig. 3 was performed using a Gaussian slit function with the full width at the half maximum of 0.24 nm corresponding to the spectral resolution of the SCIAMACHY instrument in channel 1.

In the spherical mode, photochemically active species can be accounted for, i.e., radiative transfer calculations can be performed considering solar zenith angle

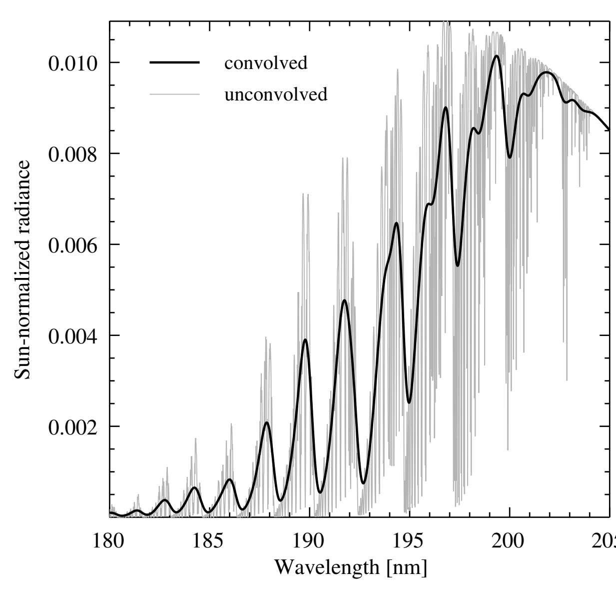

Fig. 3. Backscattered solar radiance in nadir viewing geometry.

dependent vertical distributions of atmospheric trace gases instead of using fixed vertical profiles in the entire atmosphere. Figure 4 shows a comparison of OClO slant columns appropriate to ground-based zenith-sky measurements including and neglecting the dependence of the OClO vertical distribution on the solar zenith angle. As clearly seen, due to the strong dependence of the OClO amount on the solar zenith angle the slant columns modeled assuming a fixed vertical distribution of OCLO in the atmosphere can differ much from the photochemical values.

Inelastic rotational Raman scattering (Vountas et al., 1998) can also be considered in the framework of the SCIATRAN 2.0 radiative transfer model at any supported viewing geometry. The left plot in Fig. 5 shows an example of a Ring spectrum which is obtained as a difference between logarithms of radiancies calculated including and neglecting the rotational Raman scattering (RRS), denoted I^{RRS} and I^0, respectively, i.e., $R = \ln I^{RRS} - \ln I^0$. The spectrum was calculated in a non-absorbing atmosphere in limb viewing geometry at 20 km tangent height at a solar zenith angle of 40°. The right plot in Fig. 5 shows the absolute difference between the Ring spectra calculated in nadir and limb geometry. As seen from the plots, the difference is one order of magnitude smaller than the Ring spectrum itself and has a similar spectral behavior.

In the plane-parallel mode clouds can be accounted for either using the internal cloud data base computed for various cloud droplet size distributions employing the Mie theory or supplying user-defined cloud optical parameters. An extremely fast algorithm based on the asymptotic radiative transfer theory (Kokhanovsky and Rozanov, 2004) is implemented to calculate the reflected radiance in a cloudy atmosphere within "line-absorber" (O_2, H_2O, etc.) spectral bands. The upper plot in Fig. 6 shows the reflection function, i.e., the sun-normalized radiance divided by the cosine of the solar zenith angle, simulated with SCIATRAN in the oxygen A-band spectral region in nadir viewing geometry at a solar zenith angle of 60° in a presence of cloud. The cloud was placed between between 500 and 1000 m and assumed to have the optical depth of 20. The cloud C.1 droplet size distribution (Kokhanovsky, 2004) was used to calculate the cloud phase function. The lower plot in Fig. 6 shows the percentage difference between SCIATRAN results and the reflection function obtained employing the DISORT model (Kylling and Mayer, 1993–2004; Stamnes et al., 1988). As clearly seen, the models are typically in agreement within 0.2% differing by at most 0.45%.

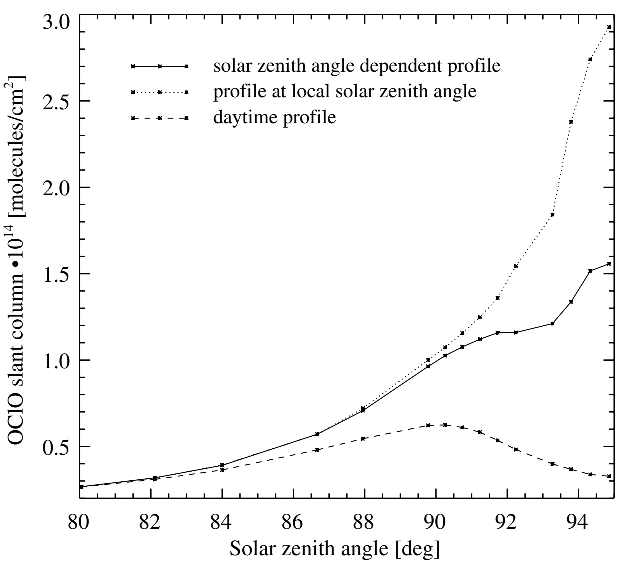

Fig. 4. OClO slant columns for ground-based zenith-sky measurements including and neglecting the dependence of OClO vertical distribution on the solar zenith angle.

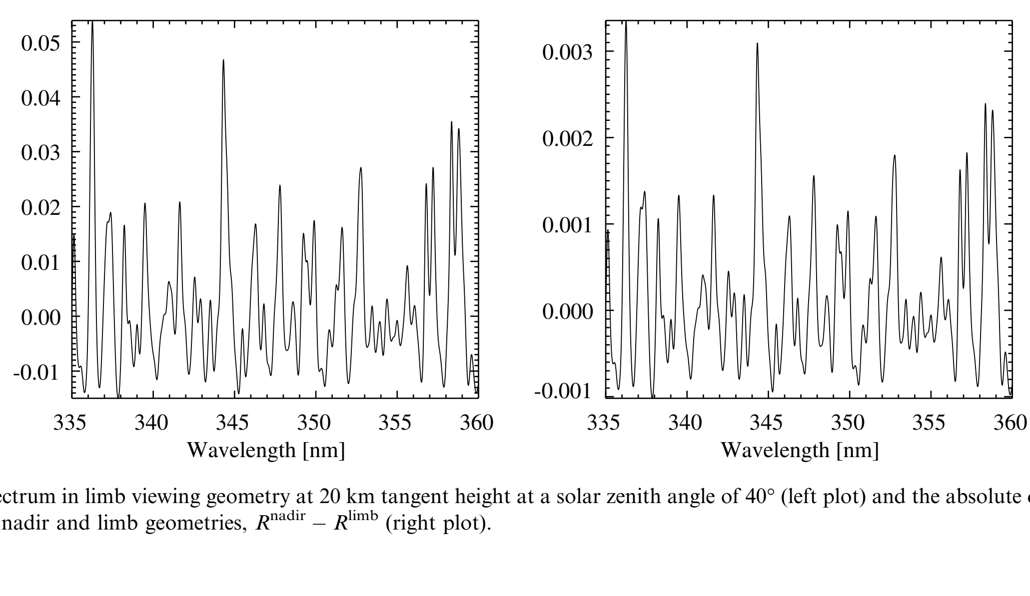

Fig. 5. Ring spectrum in limb viewing geometry at 20 km tangent height at a solar zenith angle of 40° (left plot) and the absolute difference between Ring spectra in nadir and limb geometries, $R^{nadir} - R^{limb}$ (right plot).

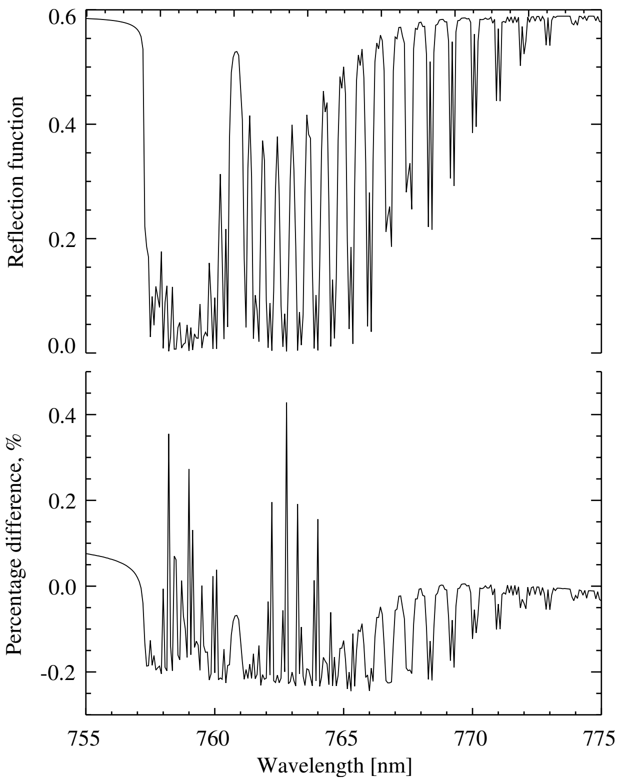

Fig. 6. Reflection function in the oxygen A-band spectral region in nadir viewing geometry at a solar zenith angle of 60° in a presence of cloud (upper plot) and the percentage difference between SCIATRAN and DISORT results (lower plot). The cloud was placed between between 500 and 1000 m and assumed to have the optical depth of 20.

3. Conclusion

The latest version of the radiative transfer model SCIATRAN has been discussed which is suitable to solve almost any scientific task related to measurements of the scattered solar radiation in the Earth's atmosphere by means of satellite, ground-based, or air-borne instruments in UV–Vis–NIR spectral region. The program is freely available for non-commercial scientific applications (http://www.iup.physik.uni-bremen.de/sciatran). The work on the polarization is currently in progress.

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